Fourier integral theorem & Gaussian function

$$\delta(x-x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{\pm i(x-x')k}\, dk$$

This is the Dirac deltafunction.

~~Since~~

$$f(x) = \int_{-\infty}^{\infty} \delta(x-x')\, f(x')\, dx' \rightarrow \text{using the Dirac } \delta \text{ function transformation integral}$$

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\pm ik(x-x')}\, f(x')\, dx'\, dk$$

we define a new value

$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx} f(x)\, dx$$

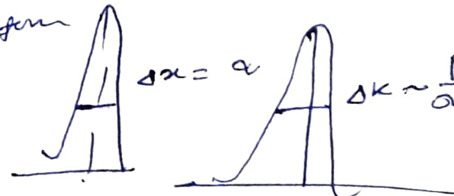
$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\, F(k)\, dk.$$

Consider the gaussian wave function

$$f(x) = A e^{-x^2/2a^2}$$

$$\xleftarrow{\text{1 2R Fourier transform}}$$

$$F(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} A e^{-ikx} e^{-x^2/2a^2}\, dx$$



$\Delta x \Delta k \approx 1$

using the identity

$$\int_{-\infty}^{\infty} e^{-\alpha x^2 + \beta x}\, dx = \sqrt{\frac{\pi}{\alpha}}\exp\left(\frac{\beta^2}{4\alpha}\right) \qquad \alpha > 0$$

$$F(k) = Aa\, e^{-\frac{k^2}{2a^2}}$$

$\longrightarrow$ F transform of a Gaussian ~~wave~~ ~~pad~~ function is also gaussian.

General sol^n of Schrodinger equation for free particle

$$\Psi(x,t) = \psi(x)\,\chi(t)$$

$$\cancel{\chi(t) = -\frac{iE}{\hbar}t}$$

$$\chi(t) = A\,e^{-\frac{i}{\hbar}Et} \longrightarrow (1)$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{p^2}{\hbar}\psi(x) = 0$$

$$\therefore \psi(x) = \text{Const}\; e^{\frac{i}{\hbar}px} \qquad p = \sqrt{2mE}.$$

Real

$E \to$ always +ve

$p \to$ ~~real and~~ real

$-\infty$ to $-\infty$

$$\psi_p(x) = \cancel{\frac{1}{\sqrt{2m\hbar}}}\;\frac{1}{\sqrt{2\pi\hbar}}\,e^{\frac{i}{\hbar}px}$$

$$\int \psi_p^*(x)\,\psi_{p'}(x)\,dx = \delta(p-p')$$

$$\langle p\rangle = \int \quad dx = \int_{-\infty}^{\infty} |a(p)|^2\,dp$$

$$\langle p^2\rangle = \int p^2 |a(p)|^2\,dp$$

$$\psi_p(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\,e^{\frac{i}{\hbar}(px-Et)}.$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\,e^{\frac{i}{\hbar}\left(px-\frac{p^2}{2m}t\right)}$$

$$\psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} a(p)\,e^{\frac{i}{\hbar}(px)}\,dp$$

for $+p \rightarrow$ along +ve

for $-p$ . . along −ve.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} a(p)\,e^{\frac{i}{\hbar}\left(px-\frac{p^2}{2m}t\right)}. \longrightarrow$$

$$a_p = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,0)\,e^{-\frac{i}{\hbar}px}\,dx$$

Evaluation of one D. wave packet.

$$\int_{-\infty} |\psi(x,0)|^2 = 1$$

$$\therefore \int_{-\infty}^{\infty} |\psi(x,t)|^2 = 0$$

The time evaluation of the centre of the wave packet

$$\langle x\rangle = \int_{-\infty}^{\infty} x\,|\psi(x,t)|^2\,dx$$

$$\langle x^2\rangle = \int_{-\infty}^{\infty} x^2\,|\psi(x,t)|^2\,dx.$$

Fourier Transformation and Momentum Space wave function.

The Dirac delta function can be expressed in the integral form

$$\delta(x-x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{\pm ki(x-x')}\, dk \quad \text{—— (1)}$$

Since

$$f(x) = \int_{-\infty}^{\infty} \delta(x-x')\, f(x')\, dx'$$

$$\therefore\ f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\pm i(x-x')k} f(x')\, dx'\, dk$$

From this we define

$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx \longrightarrow (2)$$

Then

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk \longrightarrow (3)$$

Equation (2) and (3) are combindly known as Fourier ~~transformation~~ Integral ~~transforma~~ Theorem.

The equation (2) and (3) are valid under the following condition.

(i) The function $f(x)$ must be a single valued function of the real variable x, in the range $-\infty < x < \infty$.

(ii) The integral $\int_{-\infty}^{\infty} |f(x)|\, dx$ must exist.

Q. Consider a Gaussian function given by

$f(x) = A e^{-x^2/2a^2}$

Calculate the Fourier transform of the given function.

$$F(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2a^2} e^{-ikx} \, dx \longrightarrow (1)$$

We have the identity $\int_{-\infty}^{\infty} e^{-\alpha x^2 \mp \beta x} \, dx$

$$= \sqrt{\frac{\pi}{\alpha}} \exp\left[\frac{\beta^2}{4\alpha}\right] \quad Re\,\alpha > 0$$

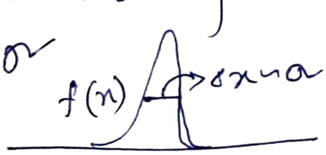
using the identity in equation (1) $\alpha = \frac{1}{2a^2}$, ~~β~~
$\beta = -ik$

$$F(k) = \frac{A}{\sqrt{2\pi}} \times \sqrt{\frac{\pi}{1/2a^2}} \exp\left[\frac{-k^2}{4 \cdot 1/2a^2}\right]$$

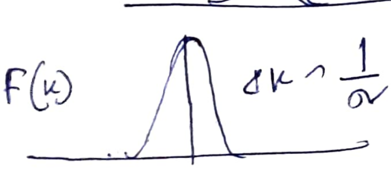
$$= A a \exp\left(\frac{-k^2 a^2}{2}\right) \longrightarrow (2)$$

From equation (2) we see that $F(k)$ is also Gaussian. So the Fourier transform of a Gaussian is a gaussain.

The Gaussian function has a spatial width $\delta x \sim a$



$\therefore \delta x \, \delta k \sim 1$



This is the general characteristics of a Fourier transformation pair.

Significance of Momentum wave function.

We have represented the wave function as the superposition of infinite number of plane waves ~~a(p)~~ as $a(p)$ as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(p)\, e^{\frac{i}{\hbar}(px - Et)}\, dp$$

In 3D

$$\psi(r,t) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} a(p)\, e^{\frac{i}{\hbar}(p.r - Et)}\, dp$$

$a(p)$ is the momentum wavefunction which is also the amplitude of the particular plane wave corresponding to a definite value of p.

Now we wish to find what p is represented in $a(p)$ or $e^{\frac{i}{\hbar}(p.r)}$

To have this we operate momentum operator $-i\hbar\nabla$ on $e^{\frac{i}{\hbar}p.r}$

$$-i\hbar\nabla\left(e^{\frac{i}{\hbar}p.r}\right) = (-i\hbar)\left(\frac{i}{\hbar}p\right) e^{\frac{i}{\hbar}p.r}$$

$$\Rightarrow -i\hbar\nabla\left(e^{\frac{i}{\hbar}p.r}\right) = p\, e^{\frac{i}{\hbar}(p.r)}$$

which is an eigen value equation for the momentum operator, indicating that $e^{\frac{i}{\hbar}p.r}$ is an eigen function of the momentum operator.

with eigen value P.

We conclude therefore that the possible momenta are given by p and the momentum eigenfunctions will depend on the value of P.

Any one of ~~these can~~ them can be represented as $a(p)\, e^{\frac{i}{\hbar} P.r}$. Therefore the momentum ~~eigenfunction~~ wavefunction $a(p)$ that we have defined are the amplitude of all possible momentum eigen functions, that superpose on the wave function $\psi(r,t)$.

The Commutator

The commutator of two operators $\hat{A}$ & $\hat{B}$ is represented by the relation $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

If the commutator of two operators is non zero, Then the ~~two opera~~ eigen values corresponding to the two operators can not be measured simultaneously. The nonzero commutator of two operators means that They are following the uncertainty relation of Heisenberg.